

Day : Tuesday  
Date: 12/11/2007

Time: 17:07:29

PALM INTRANET

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f6

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STW

(FILE 'HOME' ENTERED AT 13:22:50 ON 11 DEC 2007)

fr

FILE 'REGISTRY' ENTERED AT 13:22:59 ON 11 DEC 2007

L1 STRUCTURE UPLOADED

L2 0 S L1 SSS SAM

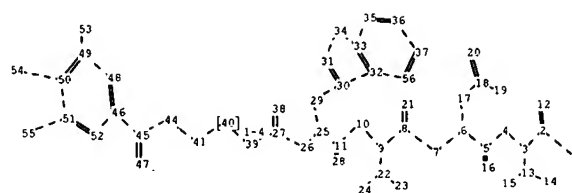
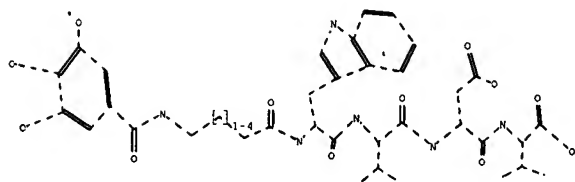
L3 3 S L1 SSS FULL

peptide 28-79

FILE 'CAPLUS, MEDLINE' ENTERED AT 13:25:10 ON 11 DEC 2007

L4 2 S L3

fr



## chain nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21  
22 23 24 25 26 27 28 29 38 39 40 41 44 45 47 53 54 55

## ring nodes :

30 31 32 33 34 35 36 37 46 48 49 50 51 52 56

## chain bonds :

1-2 2-3 2-12 3-4 3-13 4-5 5-6 5-16 6-7 6-17 7-8 8-9 8-21 9-10  
9-22 10-11 11-25 11-28 13-14 13-15 17-18 18-19 18-20 22-23 22-24  
25-26 25-29 26-27 27-38 27-39 29-30 39-40 40-41 41-44 44-45 45-46  
45-47 49-53 50-54 51-55

## ring bonds :

30-31 30-32 31-34 32-33 32-56 33-34 33-35 35-36 36-37 37-56 46-48  
46-52 48-49 49-50 50-51 51-52

## exact/norm bonds :

1-2 2-3 2-12 3-4 3-13 4-5 5-6 5-16 6-7 6-17 7-8 8-9 8-21 9-10  
9-22 10-11 11-25 11-28 13-14 13-15 17-18 18-19 18-20 22-23 22-24  
25-26 25-29 26-27 27-38 27-39 29-30 30-31 30-32 31-34 32-56 33-34  
33-35 36-37 39-40 40-41 41-44 44-45 45-46 45-47 46-52 48-49 49-53  
50-51 50-54 51-55

## normalized bonds :

32-33 35-36 37-56 46-48 49-50 51-52

## Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS  
9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS  
16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS  
23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS  
30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom  
38:CLASS 39:CLASS 40:CLASS 41:CLASS 44:CLASS 45:CLASS 46:Atom  
47:CLASS 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:CLASS 54:CLASS  
55:CLASS 56:Atom

STW for

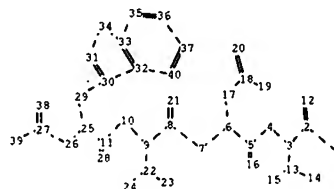
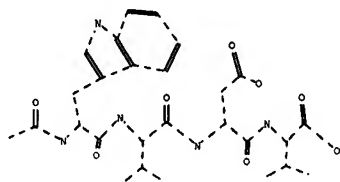
FILE 'REGISTRY' ENTERED AT 15:40:54 ON 11 DEC 2007

L1           STRUCTURE UPLOADED  
L2           1 S L1 SSS SAM  
L3           46 S L1 SSS FULL  
L4           0 S L3 AND GALLIC  
L5           4 S L3 AND TRIHYDROX?  
L6           0 S L3 AND POLYHYDROX?  
L7           0 S L3 AND AMINOBTYRIC

pytch Table 3

FILE 'CAPLUS' ENTERED AT 15:44:13 ON 11 DEC 2007

L8           2 S L5  
L9           9 S L3  
L10          7 S L9 NOT L8



chain nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21  
22 23 24 25 26 27 28 29 38 39

ring nodes :

30 31 32 33 34 35 36 37 40

chain bonds :

1-2 2-3 2-12 3-4 3-13 4-5 5-6 5-16 6-7 6-17 7-8 8-9 8-21 9-10  
9-22 10-11 11-25 11-28 13-14 13-15 17-18 18-19 18-20 22-23 22-24  
25-26 25-29 26-27 27-38 27-39 29-30

ring bonds :

30-31 30-32 31-34 32-33 32-40 33-34 33-35 35-36 36-37 37-40

exact/norm bonds :

1-2 2-3 2-12 3-4 3-13 4-5 5-6 5-16 6-7 6-17 7-8 8-9 8-21 9-10  
9-22 10-11 11-25 11-28 13-14 13-15 17-18 18-19 18-20 22-23 22-24  
25-26 25-29 26-27 27-38 27-39 29-30 30-31 30-32 31-34 32-40 33-34  
33-35 36-37

normalized bonds :

32-33 35-36 37-40

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS  
9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS  
16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS  
23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS  
30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom  
38:CLASS 39:CLASS 40:Atom